Experimental and *ab-initio* study of electric field effects in GaN/AlN multi-quantum-wells at ambient and high hydrostatic pressure

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The emission properties of nitride quantum heterostructures are strongly related to built-in electric fields caused by the spontaneous and piezoelectric polarizations characteristic for wurtzite structure. In this work we report on the correlation of ambient and high-pressure photoluminescence (PL) study of GaN/AlN multi-quantum-wells (MQWs) with *ab initio* calculations of their electronic (band structure, density of states) and optical properties (emission energies and their pressure derivatives, oscillator strength). The study was performed on GaN/AlN MQWs with various well thicknesses synthesized by plasma-assisted molecular-beam epitaxy on AlN-on-sapphire substrates. The quality of the structures was validated by X-ray diffraction (XRD) and transmission electron microscopy (TEM). PL measurements as a function of the hydrostatic pressure were conducted in a diamond anvil cell. The optical properties of the MQWs were strongly affected by the quantum confined Stark effect stemming from the polarization-induced internal electric fields. Therefore, the ambient pressure PL peak energies decreased by over 1 eV with QW thicknesses increasing from 1 nm up to 6 nm [1]. Furthermore, the respective PL decay times increased from about 1 ns up to 10^4 ns, exhibiting changes of dynamics characteristic of strong built-in electric field. The pressure coefficients of the PL energy were significantly reduced in the MQWs as compared to bulk AlN and GaN crystals, and they strongly depended on geometric factors such as the thickness of the wells and barriers.

The transition energies, their pressure dependences and oscillator strengths were modelled for tetragonally strained structures of the same geometry using a full tensorial representation of the strain in the MQWs under external pressure. The same MQWs were also simulated directly using density functional theory (DFT) calculations [2]. The good agreement between these two approaches and the experimental results indicates that the nonlinear effects induced by the tetragonal strain related to the lattice mismatch between the substrate and the MQWs are responsible for the drastic decrease of the pressure coefficients observed experimentally.

Acknowledgements: The authors acknowledge support of the Polish National Science Centre by grant No. DEC-2012/05/B/ST3/03113.

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